



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:22 PM UTC

PDB ID : 6NQN / pdb_00006nqn
Title : Crystal structure of fast switching M159T mutant of fluorescent protein Dronpa (Dronpa2), Y63(3-BrY)
Authors : Lin, C.-Y.; Romei, M.G.; Mathews, I.I.; Boxer, S.G.
Deposited on : 2019-01-21
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

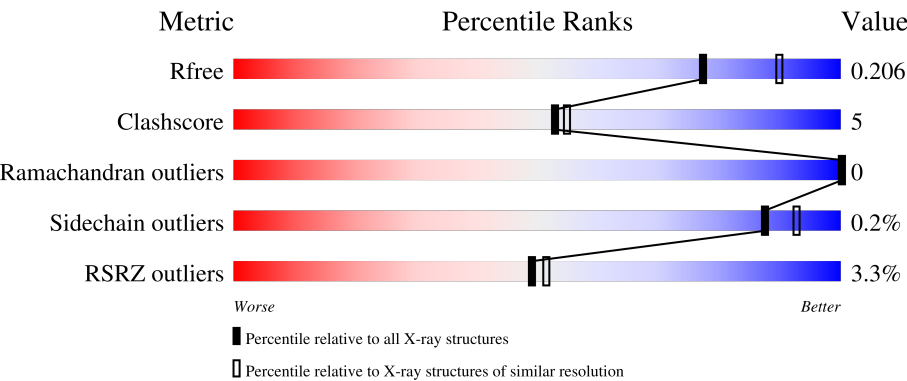
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	255	4% 79% 6% 14%
1	B	255	3% 77% 8% 15%
1	C	255	2% 75% 10% 14%
1	D	255	3% 80% 5% 13%
1	E	255	2% 79% 5% 15%

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Mol	Chain	Length	Quality of chain
1	F	255	2% 78% 7% • 15%
1	G	255	4% 76% 9% • 14%
1	H	255	2% 77% 7% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15184 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	Br	C	N	O	S	0	2	0
			1757	1	1120	295	332	9			
1	B	217	Total	Br	C	N	O	S	0	2	0
			1752	1	1118	298	326	9			
1	C	219	Total	Br	C	N	O	S	0	2	0
			1773	1	1131	297	334	10			
1	D	221	Total	Br	C	N	O	S	0	2	0
			1773	1	1131	298	334	9			
1	E	216	Total	Br	C	N	O	S	0	2	0
			1748	1	1115	294	329	9			
1	F	217	Total	Br	C	N	O	S	0	2	0
			1753	1	1119	298	326	9			
1	G	219	Total	Br	C	N	O	S	0	2	0
			1763	1	1126	295	332	9			
1	H	217	Total	Br	C	N	O	S	0	3	0
			1759	1	1120	301	328	9			

There are 328 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	GLY	-	expression tag	UNP Q5TLG6
A	-26	SER	-	expression tag	UNP Q5TLG6
A	-25	SER	-	expression tag	UNP Q5TLG6
A	-24	HIS	-	expression tag	UNP Q5TLG6
A	-23	HIS	-	expression tag	UNP Q5TLG6
A	-22	HIS	-	expression tag	UNP Q5TLG6
A	-21	HIS	-	expression tag	UNP Q5TLG6
A	-20	HIS	-	expression tag	UNP Q5TLG6
A	-19	HIS	-	expression tag	UNP Q5TLG6
A	-18	SER	-	expression tag	UNP Q5TLG6
A	-17	SER	-	expression tag	UNP Q5TLG6
A	-16	GLY	-	expression tag	UNP Q5TLG6
A	-15	LEU	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	VAL	-	expression tag	UNP Q5TLG6
A	-13	PRO	-	expression tag	UNP Q5TLG6
A	-12	GLY	-	expression tag	UNP Q5TLG6
A	-11	GLY	-	expression tag	UNP Q5TLG6
A	-10	SER	-	expression tag	UNP Q5TLG6
A	-9	HIS	-	expression tag	UNP Q5TLG6
A	-8	MET	-	expression tag	UNP Q5TLG6
A	-7	VAL	-	expression tag	UNP Q5TLG6
A	-6	SER	-	expression tag	UNP Q5TLG6
A	-5	LYS	-	expression tag	UNP Q5TLG6
A	-4	GLY	-	expression tag	UNP Q5TLG6
A	-3	GLU	-	expression tag	UNP Q5TLG6
A	-2	GLU	-	expression tag	UNP Q5TLG6
A	-1	ASN	-	expression tag	UNP Q5TLG6
A	0	ASN	-	expression tag	UNP Q5TLG6
A	1	MET	-	expression tag	UNP Q5TLG6
A	2	ALA	-	expression tag	UNP Q5TLG6
A	63	KZ4	CYS	chromophore	UNP Q5TLG6
A	63	KZ4	TYR	chromophore	UNP Q5TLG6
A	63	KZ4	GLY	chromophore	UNP Q5TLG6
A	159	THR	MET	engineered mutation	UNP Q5TLG6
A	218	GLY	GLU	engineered mutation	UNP Q5TLG6
A	224	MET	-	expression tag	UNP Q5TLG6
A	225	ASP	-	expression tag	UNP Q5TLG6
A	226	GLU	-	expression tag	UNP Q5TLG6
A	227	LEU	-	expression tag	UNP Q5TLG6
A	228	TYR	-	expression tag	UNP Q5TLG6
A	229	LYS	-	expression tag	UNP Q5TLG6
B	-27	GLY	-	expression tag	UNP Q5TLG6
B	-26	SER	-	expression tag	UNP Q5TLG6
B	-25	SER	-	expression tag	UNP Q5TLG6
B	-24	HIS	-	expression tag	UNP Q5TLG6
B	-23	HIS	-	expression tag	UNP Q5TLG6
B	-22	HIS	-	expression tag	UNP Q5TLG6
B	-21	HIS	-	expression tag	UNP Q5TLG6
B	-20	HIS	-	expression tag	UNP Q5TLG6
B	-19	HIS	-	expression tag	UNP Q5TLG6
B	-18	SER	-	expression tag	UNP Q5TLG6
B	-17	SER	-	expression tag	UNP Q5TLG6
B	-16	GLY	-	expression tag	UNP Q5TLG6
B	-15	LEU	-	expression tag	UNP Q5TLG6
B	-14	VAL	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	PRO	-	expression tag	UNP Q5TLG6
B	-12	GLY	-	expression tag	UNP Q5TLG6
B	-11	GLY	-	expression tag	UNP Q5TLG6
B	-10	SER	-	expression tag	UNP Q5TLG6
B	-9	HIS	-	expression tag	UNP Q5TLG6
B	-8	MET	-	expression tag	UNP Q5TLG6
B	-7	VAL	-	expression tag	UNP Q5TLG6
B	-6	SER	-	expression tag	UNP Q5TLG6
B	-5	LYS	-	expression tag	UNP Q5TLG6
B	-4	GLY	-	expression tag	UNP Q5TLG6
B	-3	GLU	-	expression tag	UNP Q5TLG6
B	-2	GLU	-	expression tag	UNP Q5TLG6
B	-1	ASN	-	expression tag	UNP Q5TLG6
B	0	ASN	-	expression tag	UNP Q5TLG6
B	1	MET	-	expression tag	UNP Q5TLG6
B	2	ALA	-	expression tag	UNP Q5TLG6
B	63	KZ4	CYS	chromophore	UNP Q5TLG6
B	63	KZ4	TYR	chromophore	UNP Q5TLG6
B	63	KZ4	GLY	chromophore	UNP Q5TLG6
B	159	THR	MET	engineered mutation	UNP Q5TLG6
B	218	GLY	GLU	engineered mutation	UNP Q5TLG6
B	224	MET	-	expression tag	UNP Q5TLG6
B	225	ASP	-	expression tag	UNP Q5TLG6
B	226	GLU	-	expression tag	UNP Q5TLG6
B	227	LEU	-	expression tag	UNP Q5TLG6
B	228	TYR	-	expression tag	UNP Q5TLG6
B	229	LYS	-	expression tag	UNP Q5TLG6
C	-27	GLY	-	expression tag	UNP Q5TLG6
C	-26	SER	-	expression tag	UNP Q5TLG6
C	-25	SER	-	expression tag	UNP Q5TLG6
C	-24	HIS	-	expression tag	UNP Q5TLG6
C	-23	HIS	-	expression tag	UNP Q5TLG6
C	-22	HIS	-	expression tag	UNP Q5TLG6
C	-21	HIS	-	expression tag	UNP Q5TLG6
C	-20	HIS	-	expression tag	UNP Q5TLG6
C	-19	HIS	-	expression tag	UNP Q5TLG6
C	-18	SER	-	expression tag	UNP Q5TLG6
C	-17	SER	-	expression tag	UNP Q5TLG6
C	-16	GLY	-	expression tag	UNP Q5TLG6
C	-15	LEU	-	expression tag	UNP Q5TLG6
C	-14	VAL	-	expression tag	UNP Q5TLG6
C	-13	PRO	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	GLY	-	expression tag	UNP Q5TLG6
C	-11	GLY	-	expression tag	UNP Q5TLG6
C	-10	SER	-	expression tag	UNP Q5TLG6
C	-9	HIS	-	expression tag	UNP Q5TLG6
C	-8	MET	-	expression tag	UNP Q5TLG6
C	-7	VAL	-	expression tag	UNP Q5TLG6
C	-6	SER	-	expression tag	UNP Q5TLG6
C	-5	LYS	-	expression tag	UNP Q5TLG6
C	-4	GLY	-	expression tag	UNP Q5TLG6
C	-3	GLU	-	expression tag	UNP Q5TLG6
C	-2	GLU	-	expression tag	UNP Q5TLG6
C	-1	ASN	-	expression tag	UNP Q5TLG6
C	0	ASN	-	expression tag	UNP Q5TLG6
C	1	MET	-	expression tag	UNP Q5TLG6
C	2	ALA	-	expression tag	UNP Q5TLG6
C	63	KZ4	CYS	chromophore	UNP Q5TLG6
C	63	KZ4	TYR	chromophore	UNP Q5TLG6
C	63	KZ4	GLY	chromophore	UNP Q5TLG6
C	159	THR	MET	engineered mutation	UNP Q5TLG6
C	218	GLY	GLU	engineered mutation	UNP Q5TLG6
C	224	MET	-	expression tag	UNP Q5TLG6
C	225	ASP	-	expression tag	UNP Q5TLG6
C	226	GLU	-	expression tag	UNP Q5TLG6
C	227	LEU	-	expression tag	UNP Q5TLG6
C	228	TYR	-	expression tag	UNP Q5TLG6
C	229	LYS	-	expression tag	UNP Q5TLG6
D	-27	GLY	-	expression tag	UNP Q5TLG6
D	-26	SER	-	expression tag	UNP Q5TLG6
D	-25	SER	-	expression tag	UNP Q5TLG6
D	-24	HIS	-	expression tag	UNP Q5TLG6
D	-23	HIS	-	expression tag	UNP Q5TLG6
D	-22	HIS	-	expression tag	UNP Q5TLG6
D	-21	HIS	-	expression tag	UNP Q5TLG6
D	-20	HIS	-	expression tag	UNP Q5TLG6
D	-19	HIS	-	expression tag	UNP Q5TLG6
D	-18	SER	-	expression tag	UNP Q5TLG6
D	-17	SER	-	expression tag	UNP Q5TLG6
D	-16	GLY	-	expression tag	UNP Q5TLG6
D	-15	LEU	-	expression tag	UNP Q5TLG6
D	-14	VAL	-	expression tag	UNP Q5TLG6
D	-13	PRO	-	expression tag	UNP Q5TLG6
D	-12	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	GLY	-	expression tag	UNP Q5TLG6
D	-10	SER	-	expression tag	UNP Q5TLG6
D	-9	HIS	-	expression tag	UNP Q5TLG6
D	-8	MET	-	expression tag	UNP Q5TLG6
D	-7	VAL	-	expression tag	UNP Q5TLG6
D	-6	SER	-	expression tag	UNP Q5TLG6
D	-5	LYS	-	expression tag	UNP Q5TLG6
D	-4	GLY	-	expression tag	UNP Q5TLG6
D	-3	GLU	-	expression tag	UNP Q5TLG6
D	-2	GLU	-	expression tag	UNP Q5TLG6
D	-1	ASN	-	expression tag	UNP Q5TLG6
D	0	ASN	-	expression tag	UNP Q5TLG6
D	1	MET	-	expression tag	UNP Q5TLG6
D	2	ALA	-	expression tag	UNP Q5TLG6
D	63	KZ4	CYS	chromophore	UNP Q5TLG6
D	63	KZ4	TYR	chromophore	UNP Q5TLG6
D	63	KZ4	GLY	chromophore	UNP Q5TLG6
D	159	THR	MET	engineered mutation	UNP Q5TLG6
D	218	GLY	GLU	engineered mutation	UNP Q5TLG6
D	224	MET	-	expression tag	UNP Q5TLG6
D	225	ASP	-	expression tag	UNP Q5TLG6
D	226	GLU	-	expression tag	UNP Q5TLG6
D	227	LEU	-	expression tag	UNP Q5TLG6
D	228	TYR	-	expression tag	UNP Q5TLG6
D	229	LYS	-	expression tag	UNP Q5TLG6
E	-27	GLY	-	expression tag	UNP Q5TLG6
E	-26	SER	-	expression tag	UNP Q5TLG6
E	-25	SER	-	expression tag	UNP Q5TLG6
E	-24	HIS	-	expression tag	UNP Q5TLG6
E	-23	HIS	-	expression tag	UNP Q5TLG6
E	-22	HIS	-	expression tag	UNP Q5TLG6
E	-21	HIS	-	expression tag	UNP Q5TLG6
E	-20	HIS	-	expression tag	UNP Q5TLG6
E	-19	HIS	-	expression tag	UNP Q5TLG6
E	-18	SER	-	expression tag	UNP Q5TLG6
E	-17	SER	-	expression tag	UNP Q5TLG6
E	-16	GLY	-	expression tag	UNP Q5TLG6
E	-15	LEU	-	expression tag	UNP Q5TLG6
E	-14	VAL	-	expression tag	UNP Q5TLG6
E	-13	PRO	-	expression tag	UNP Q5TLG6
E	-12	GLY	-	expression tag	UNP Q5TLG6
E	-11	GLY	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	SER	-	expression tag	UNP Q5TLG6
E	-9	HIS	-	expression tag	UNP Q5TLG6
E	-8	MET	-	expression tag	UNP Q5TLG6
E	-7	VAL	-	expression tag	UNP Q5TLG6
E	-6	SER	-	expression tag	UNP Q5TLG6
E	-5	LYS	-	expression tag	UNP Q5TLG6
E	-4	GLY	-	expression tag	UNP Q5TLG6
E	-3	GLU	-	expression tag	UNP Q5TLG6
E	-2	GLU	-	expression tag	UNP Q5TLG6
E	-1	ASN	-	expression tag	UNP Q5TLG6
E	0	ASN	-	expression tag	UNP Q5TLG6
E	1	MET	-	expression tag	UNP Q5TLG6
E	2	ALA	-	expression tag	UNP Q5TLG6
E	63	KZ4	CYS	chromophore	UNP Q5TLG6
E	63	KZ4	TYR	chromophore	UNP Q5TLG6
E	63	KZ4	GLY	chromophore	UNP Q5TLG6
E	159	THR	MET	engineered mutation	UNP Q5TLG6
E	218	GLY	GLU	engineered mutation	UNP Q5TLG6
E	224	MET	-	expression tag	UNP Q5TLG6
E	225	ASP	-	expression tag	UNP Q5TLG6
E	226	GLU	-	expression tag	UNP Q5TLG6
E	227	LEU	-	expression tag	UNP Q5TLG6
E	228	TYR	-	expression tag	UNP Q5TLG6
E	229	LYS	-	expression tag	UNP Q5TLG6
F	-27	GLY	-	expression tag	UNP Q5TLG6
F	-26	SER	-	expression tag	UNP Q5TLG6
F	-25	SER	-	expression tag	UNP Q5TLG6
F	-24	HIS	-	expression tag	UNP Q5TLG6
F	-23	HIS	-	expression tag	UNP Q5TLG6
F	-22	HIS	-	expression tag	UNP Q5TLG6
F	-21	HIS	-	expression tag	UNP Q5TLG6
F	-20	HIS	-	expression tag	UNP Q5TLG6
F	-19	HIS	-	expression tag	UNP Q5TLG6
F	-18	SER	-	expression tag	UNP Q5TLG6
F	-17	SER	-	expression tag	UNP Q5TLG6
F	-16	GLY	-	expression tag	UNP Q5TLG6
F	-15	LEU	-	expression tag	UNP Q5TLG6
F	-14	VAL	-	expression tag	UNP Q5TLG6
F	-13	PRO	-	expression tag	UNP Q5TLG6
F	-12	GLY	-	expression tag	UNP Q5TLG6
F	-11	GLY	-	expression tag	UNP Q5TLG6
F	-10	SER	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-9	HIS	-	expression tag	UNP Q5TLG6
F	-8	MET	-	expression tag	UNP Q5TLG6
F	-7	VAL	-	expression tag	UNP Q5TLG6
F	-6	SER	-	expression tag	UNP Q5TLG6
F	-5	LYS	-	expression tag	UNP Q5TLG6
F	-4	GLY	-	expression tag	UNP Q5TLG6
F	-3	GLU	-	expression tag	UNP Q5TLG6
F	-2	GLU	-	expression tag	UNP Q5TLG6
F	-1	ASN	-	expression tag	UNP Q5TLG6
F	0	ASN	-	expression tag	UNP Q5TLG6
F	1	MET	-	expression tag	UNP Q5TLG6
F	2	ALA	-	expression tag	UNP Q5TLG6
F	63	KZ4	CYS	chromophore	UNP Q5TLG6
F	63	KZ4	TYR	chromophore	UNP Q5TLG6
F	63	KZ4	GLY	chromophore	UNP Q5TLG6
F	159	THR	MET	engineered mutation	UNP Q5TLG6
F	218	GLY	GLU	engineered mutation	UNP Q5TLG6
F	224	MET	-	expression tag	UNP Q5TLG6
F	225	ASP	-	expression tag	UNP Q5TLG6
F	226	GLU	-	expression tag	UNP Q5TLG6
F	227	LEU	-	expression tag	UNP Q5TLG6
F	228	TYR	-	expression tag	UNP Q5TLG6
F	229	LYS	-	expression tag	UNP Q5TLG6
G	-27	GLY	-	expression tag	UNP Q5TLG6
G	-26	SER	-	expression tag	UNP Q5TLG6
G	-25	SER	-	expression tag	UNP Q5TLG6
G	-24	HIS	-	expression tag	UNP Q5TLG6
G	-23	HIS	-	expression tag	UNP Q5TLG6
G	-22	HIS	-	expression tag	UNP Q5TLG6
G	-21	HIS	-	expression tag	UNP Q5TLG6
G	-20	HIS	-	expression tag	UNP Q5TLG6
G	-19	HIS	-	expression tag	UNP Q5TLG6
G	-18	SER	-	expression tag	UNP Q5TLG6
G	-17	SER	-	expression tag	UNP Q5TLG6
G	-16	GLY	-	expression tag	UNP Q5TLG6
G	-15	LEU	-	expression tag	UNP Q5TLG6
G	-14	VAL	-	expression tag	UNP Q5TLG6
G	-13	PRO	-	expression tag	UNP Q5TLG6
G	-12	GLY	-	expression tag	UNP Q5TLG6
G	-11	GLY	-	expression tag	UNP Q5TLG6
G	-10	SER	-	expression tag	UNP Q5TLG6
G	-9	HIS	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	MET	-	expression tag	UNP Q5TLG6
G	-7	VAL	-	expression tag	UNP Q5TLG6
G	-6	SER	-	expression tag	UNP Q5TLG6
G	-5	LYS	-	expression tag	UNP Q5TLG6
G	-4	GLY	-	expression tag	UNP Q5TLG6
G	-3	GLU	-	expression tag	UNP Q5TLG6
G	-2	GLU	-	expression tag	UNP Q5TLG6
G	-1	ASN	-	expression tag	UNP Q5TLG6
G	0	ASN	-	expression tag	UNP Q5TLG6
G	1	MET	-	expression tag	UNP Q5TLG6
G	2	ALA	-	expression tag	UNP Q5TLG6
G	63	KZ4	CYS	chromophore	UNP Q5TLG6
G	63	KZ4	TYR	chromophore	UNP Q5TLG6
G	63	KZ4	GLY	chromophore	UNP Q5TLG6
G	159	THR	MET	engineered mutation	UNP Q5TLG6
G	218	GLY	GLU	engineered mutation	UNP Q5TLG6
G	224	MET	-	expression tag	UNP Q5TLG6
G	225	ASP	-	expression tag	UNP Q5TLG6
G	226	GLU	-	expression tag	UNP Q5TLG6
G	227	LEU	-	expression tag	UNP Q5TLG6
G	228	TYR	-	expression tag	UNP Q5TLG6
G	229	LYS	-	expression tag	UNP Q5TLG6
H	-27	GLY	-	expression tag	UNP Q5TLG6
H	-26	SER	-	expression tag	UNP Q5TLG6
H	-25	SER	-	expression tag	UNP Q5TLG6
H	-24	HIS	-	expression tag	UNP Q5TLG6
H	-23	HIS	-	expression tag	UNP Q5TLG6
H	-22	HIS	-	expression tag	UNP Q5TLG6
H	-21	HIS	-	expression tag	UNP Q5TLG6
H	-20	HIS	-	expression tag	UNP Q5TLG6
H	-19	HIS	-	expression tag	UNP Q5TLG6
H	-18	SER	-	expression tag	UNP Q5TLG6
H	-17	SER	-	expression tag	UNP Q5TLG6
H	-16	GLY	-	expression tag	UNP Q5TLG6
H	-15	LEU	-	expression tag	UNP Q5TLG6
H	-14	VAL	-	expression tag	UNP Q5TLG6
H	-13	PRO	-	expression tag	UNP Q5TLG6
H	-12	GLY	-	expression tag	UNP Q5TLG6
H	-11	GLY	-	expression tag	UNP Q5TLG6
H	-10	SER	-	expression tag	UNP Q5TLG6
H	-9	HIS	-	expression tag	UNP Q5TLG6
H	-8	MET	-	expression tag	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-7	VAL	-	expression tag	UNP Q5TLG6
H	-6	SER	-	expression tag	UNP Q5TLG6
H	-5	LYS	-	expression tag	UNP Q5TLG6
H	-4	GLY	-	expression tag	UNP Q5TLG6
H	-3	GLU	-	expression tag	UNP Q5TLG6
H	-2	GLU	-	expression tag	UNP Q5TLG6
H	-1	ASN	-	expression tag	UNP Q5TLG6
H	0	ASN	-	expression tag	UNP Q5TLG6
H	1	MET	-	expression tag	UNP Q5TLG6
H	2	ALA	-	expression tag	UNP Q5TLG6
H	63	KZ4	CYS	chromophore	UNP Q5TLG6
H	63	KZ4	TYR	chromophore	UNP Q5TLG6
H	63	KZ4	GLY	chromophore	UNP Q5TLG6
H	159	THR	MET	engineered mutation	UNP Q5TLG6
H	218	GLY	GLU	engineered mutation	UNP Q5TLG6
H	224	MET	-	expression tag	UNP Q5TLG6
H	225	ASP	-	expression tag	UNP Q5TLG6
H	226	GLU	-	expression tag	UNP Q5TLG6
H	227	LEU	-	expression tag	UNP Q5TLG6
H	228	TYR	-	expression tag	UNP Q5TLG6
H	229	LYS	-	expression tag	UNP Q5TLG6

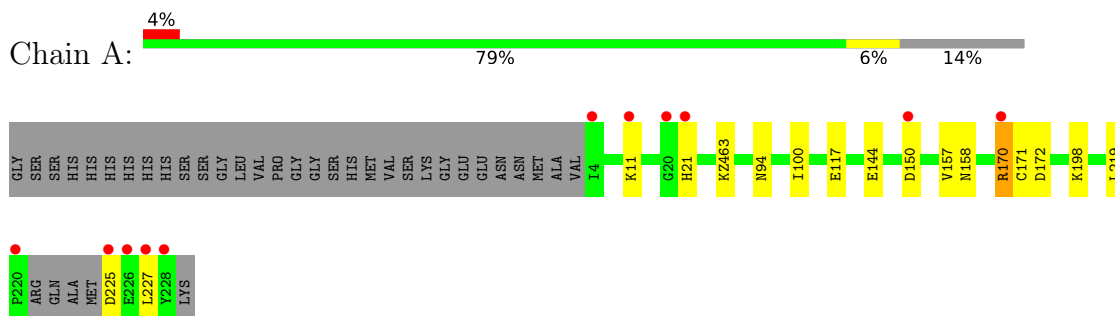
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	143	Total	O	0	0
			143	143		
2	B	142	Total	O	0	0
			142	142		
2	C	150	Total	O	0	0
			150	150		
2	D	142	Total	O	0	0
			142	142		
2	E	140	Total	O	0	0
			140	140		
2	F	151	Total	O	0	0
			151	151		
2	G	118	Total	O	0	0
			118	118		
2	H	120	Total	O	0	0
			120	120		

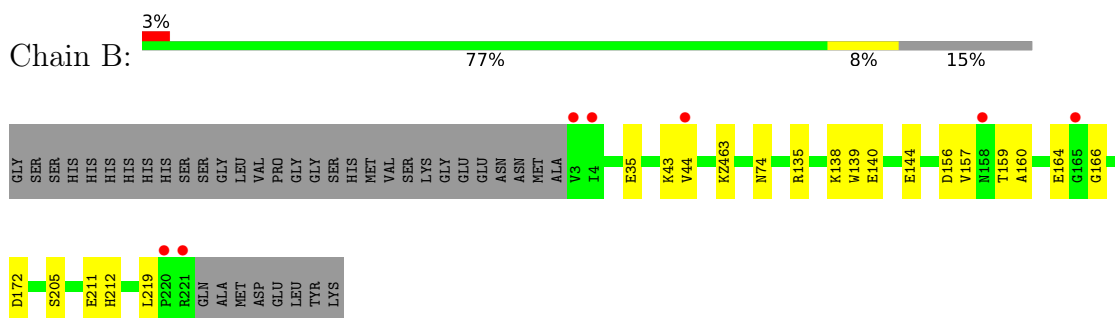
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

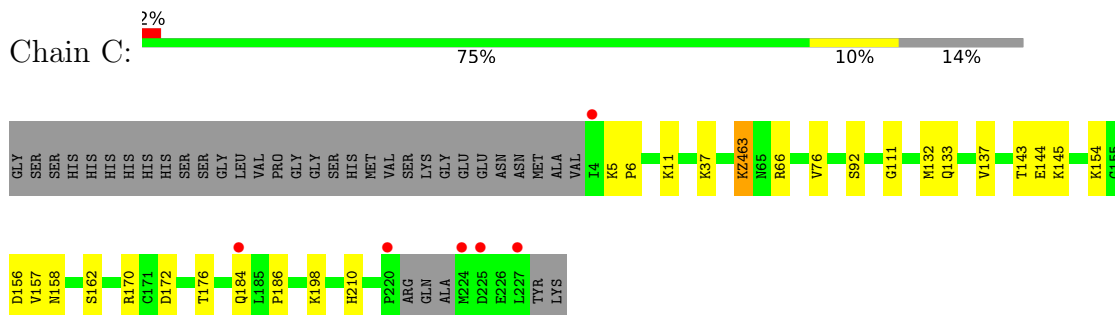
- Molecule 1: Fluorescent protein Dronpa



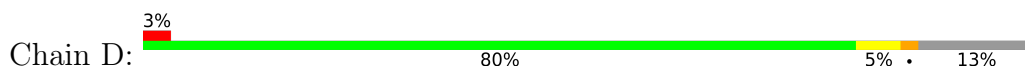
- Molecule 1: Fluorescent protein Dronpa

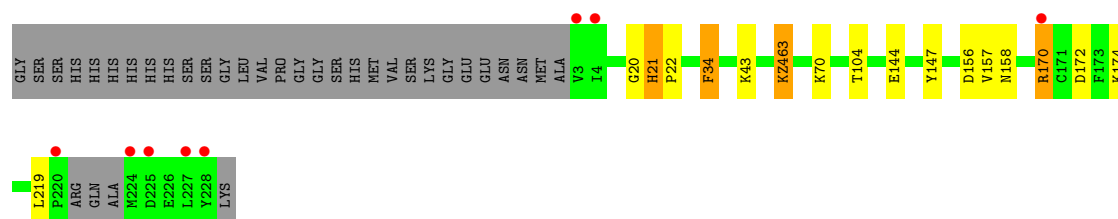


- Molecule 1: Fluorescent protein Dronpa

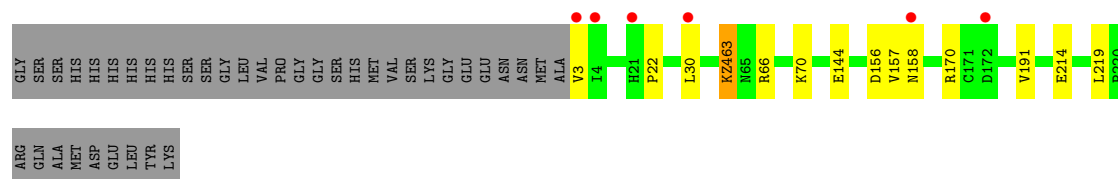
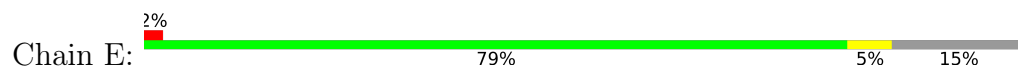


- Molecule 1: Fluorescent protein Dronpa

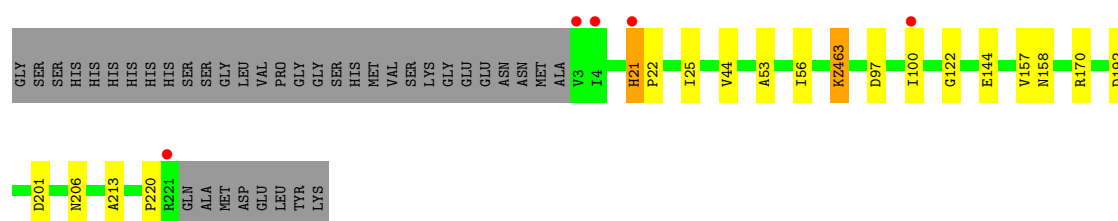
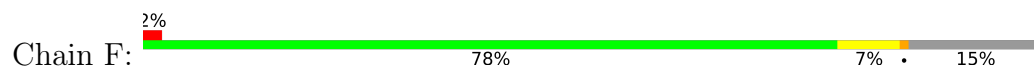




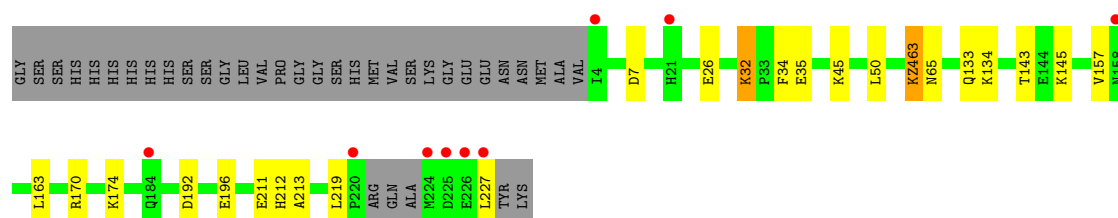
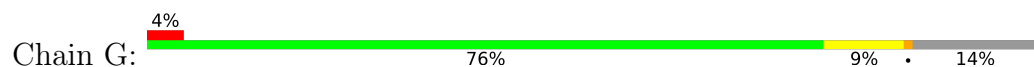
• Molecule 1: Fluorescent protein Dronpa



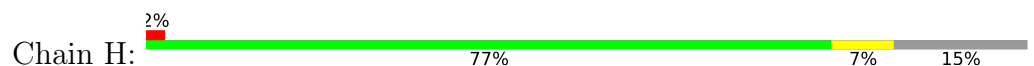
• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa



• Molecule 1: Fluorescent protein Dronpa



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.39Å 79.49Å 85.65Å 89.92° 92.40° 94.89°	Depositor
Resolution (Å)	37.61 – 2.10 37.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (37.61-2.10) 97.7 (37.61-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.13RC2_2986: ???)	Depositor
R, R_{free}	0.172 , 0.204 0.174 , 0.206	Depositor DCC
R_{free} test set	5345 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.109 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15184	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: KZ4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	2/1783 (0.1%)	0.73	8/2409 (0.3%)
1	B	0.35	0/1776	0.53	1/2399 (0.0%)
1	C	0.34	0/1796	0.60	3/2424 (0.1%)
1	D	0.33	0/1796	0.66	6/2426 (0.2%)
1	E	0.40	0/1772	0.61	1/2395 (0.0%)
1	F	0.40	0/1777	0.62	2/2401 (0.1%)
1	G	0.37	0/1786	0.63	4/2413 (0.2%)
1	H	0.40	0/1786	0.64	0/2411
All	All	0.38	2/14272 (0.0%)	0.63	25/19278 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150[A]	ASP	CA-C	5.67	1.60	1.53
1	A	150[B]	ASP	CA-C	5.67	1.60	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	21	HIS	CA-C-N	9.59	129.35	119.76
1	D	21	HIS	C-N-CA	9.59	129.35	119.76
1	A	150[A]	ASP	CA-C-O	8.31	131.47	121.08
1	A	150[B]	ASP	CA-C-O	8.31	131.47	121.08
1	A	150[A]	ASP	N-CA-C	7.36	121.62	111.90
1	A	150[B]	ASP	N-CA-C	7.36	121.62	111.90
1	A	21	HIS	CA-C-N	7.28	127.85	120.14
1	A	21	HIS	C-N-CA	7.28	127.85	120.14
1	G	32	LYS	CA-C-N	7.01	126.53	119.24
1	G	32	LYS	C-N-CA	7.01	126.53	119.24
1	F	21	HIS	CA-C-N	6.73	126.72	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	21	HIS	C-N-CA	6.73	126.72	119.78
1	D	170	ARG	N-CA-C	6.22	118.74	110.53
1	G	163	LEU	CA-C-N	6.07	129.24	120.38
1	G	163	LEU	C-N-CA	6.07	129.24	120.38
1	C	133	GLN	CA-CB-CG	-5.64	102.81	114.10
1	C	132	MET	CA-C-N	-5.31	114.16	122.65
1	C	132	MET	C-N-CA	-5.31	114.16	122.65
1	D	34	PHE	N-CA-C	5.28	117.95	111.82
1	B	74	ASN	N-CA-C	5.21	119.50	113.20
1	D	20	GLY	CA-C-N	-5.16	114.58	122.42
1	D	20	GLY	C-N-CA	-5.16	114.58	122.42
1	E	22	PRO	N-CA-C	5.11	120.21	111.68
1	A	11	LYS	CA-C-N	-5.02	114.39	122.82
1	A	11	LYS	C-N-CA	-5.02	114.39	122.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1757	0	1644	23	0
1	B	1752	0	1658	14	0
1	C	1773	0	1676	25	0
1	D	1773	0	1661	23	0
1	E	1748	0	1654	13	0
1	F	1753	0	1663	18	0
1	G	1763	0	1653	16	0
1	H	1759	0	1663	20	0
2	A	143	0	0	1	0
2	B	142	0	0	3	0
2	C	150	0	0	4	0
2	D	142	0	0	4	0
2	E	140	0	0	0	0
2	F	151	0	0	7	0
2	G	118	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	120	0	0	5	0
All	All	15184	0	13272	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASN:HB3	1:A:170:ARG:NH2	1.28	1.40
1:A:158:ASN:HB3	1:A:170:ARG:CZ	1.64	1.27
1:A:158:ASN:CB	1:A:170:ARG:HH22	1.49	1.25
1:A:158:ASN:CB	1:A:170:ARG:NH2	2.02	1.23
1:F:220:PRO:HD3	2:F:396:HOH:O	1.49	1.08
1:H:29:GLY:O	1:H:30:LEU:HD12	1.57	1.04
1:A:158:ASN:CG	1:A:170:ARG:HH22	1.74	0.94
1:G:32:LYS:HD3	1:G:35:GLU:OE1	1.71	0.91
1:B:138:LYS:NZ	1:B:139:TRP:O	2.04	0.89
1:A:158:ASN:HB3	1:A:170:ARG:NH1	1.87	0.89
1:D:158:ASN:ND2	1:D:170:ARG:HH12	1.72	0.87
1:H:29:GLY:C	1:H:30:LEU:HD12	1.99	0.85
1:C:158:ASN:CG	1:E:158:ASN:OD1	2.24	0.80
1:A:158:ASN:HB3	1:A:170:ARG:HH22	1.05	0.79
1:D:158:ASN:OD1	1:F:158:ASN:ND2	2.22	0.73
1:C:184:GLN:OE1	1:H:182:VAL:HG12	1.91	0.71
1:B:44:VAL:HG23	1:B:205:SER:HA	1.72	0.71
1:F:97:ASP:HB3	2:F:434:HOH:O	1.91	0.70
1:B:44:VAL:CG2	1:B:205:SER:HA	2.23	0.69
1:H:196:GLU:HB3	2:H:301:HOH:O	1.93	0.68
1:A:170:ARG:HG3	1:A:170:ARG:HH11	1.58	0.68
1:E:70:LYS:HB3	1:E:214:GLU:HG2	1.75	0.68
1:A:117:GLU:OE2	2:A:301:HOH:O	2.13	0.67
1:D:158:ASN:CG	1:D:170:ARG:HH12	2.01	0.67
1:G:32:LYS:HD3	1:G:35:GLU:CD	2.19	0.67
1:H:201:ASP:OD2	1:H:206:ASN:ND2	2.26	0.66
1:G:26:GLU:OE2	1:G:45:LYS:HG3	1.96	0.65
1:B:211:GLU:HG2	1:B:212:HIS:N	2.12	0.64
1:A:170:ARG:NH1	1:A:172:ASP:OD1	2.31	0.63
1:C:158:ASN:ND2	1:C:172:ASP:OD2	2.32	0.62
1:H:196:GLU:OE1	2:H:301:HOH:O	2.16	0.61
1:G:50:LEU:O	1:G:134:LYS:NZ	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ASN:ND2	1:C:172:ASP:CG	2.58	0.60
1:F:220:PRO:CD	2:F:396:HOH:O	2.25	0.60
1:F:144:GLU:HA	1:F:157:VAL:HB	1.83	0.60
1:C:156:ASP:OD1	1:E:170:ARG:NE	2.35	0.59
1:C:158:ASN:OD1	1:E:158:ASN:ND2	2.36	0.59
1:A:170:ARG:HH21	1:B:156:ASP:HB3	1.67	0.59
1:F:21:HIS:CD2	2:F:426:HOH:O	2.55	0.58
1:A:94:ASN:HA	1:A:100:ILE:HD12	1.85	0.57
1:C:158:ASN:ND2	1:E:158:ASN:OD1	2.37	0.57
1:H:144:GLU:HA	1:H:157:VAL:HB	1.85	0.57
1:C:158:ASN:HD21	1:C:172:ASP:CG	2.13	0.56
1:A:170:ARG:HH11	1:A:170:ARG:CG	2.19	0.56
1:D:174:LYS:NZ	2:F:303:HOH:O	2.37	0.56
1:B:172:ASP:OD1	2:B:301:HOH:O	2.18	0.56
1:G:170:ARG:NE	1:H:156:ASP:OD1	2.36	0.55
1:B:144:GLU:HA	1:B:157:VAL:HB	1.90	0.54
1:H:158:ASN:HB2	2:H:339:HOH:O	2.06	0.54
1:C:210:HIS:HD2	2:C:418:HOH:O	1.89	0.54
1:C:5:LYS:HG3	1:C:6:PRO:HD2	1.89	0.53
1:D:158:ASN:CG	1:F:158:ASN:ND2	2.66	0.53
1:D:158:ASN:ND2	2:D:306:HOH:O	2.42	0.53
1:D:158:ASN:HB3	1:D:170:ARG:NH2	2.23	0.52
1:G:174:LYS:NZ	2:G:302:HOH:O	2.24	0.51
1:E:144:GLU:HA	1:E:157:VAL:HB	1.92	0.51
1:A:170:ARG:HG3	1:A:171:CYS:N	2.26	0.50
1:H:29:GLY:C	1:H:30:LEU:CD1	2.80	0.50
1:G:196:GLU:OE2	1:H:221:ARG:HG2	2.10	0.50
1:F:21:HIS:HD2	2:F:426:HOH:O	1.94	0.50
1:G:143:THR:O	1:G:145:LYS:NZ	2.42	0.50
1:B:159:THR:OG1	1:B:160:ALA:N	2.43	0.50
1:D:158:ASN:ND2	1:D:170:ARG:NH1	2.53	0.50
1:D:147:TYR:CZ	1:F:170:ARG:HD3	2.47	0.49
1:D:158:ASN:HB3	1:D:170:ARG:CZ	2.42	0.49
1:G:211:GLU:HG2	1:G:212:HIS:N	2.27	0.49
1:A:158:ASN:CB	1:A:170:ARG:NH1	2.69	0.49
1:D:158:ASN:HB3	1:D:170:ARG:NH1	2.27	0.49
1:F:25:ILE:HG12	1:F:44:VAL:HG22	1.94	0.49
1:F:100:ILE:O	1:F:122:GLY:HA2	2.13	0.49
1:D:34:PHE:O	1:D:70:LYS:HG3	2.13	0.48
1:D:144:GLU:HA	1:D:157:VAL:HB	1.94	0.48
1:A:170:ARG:NH1	1:A:170:ARG:CG	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:LEU:C	1:E:30:LEU:HD12	2.39	0.48
1:B:135:ARG:NH2	2:B:306:HOH:O	2.43	0.48
1:C:143:THR:O	1:C:145:LYS:NZ	2.45	0.47
1:C:144:GLU:HA	1:C:157:VAL:HB	1.97	0.47
1:H:63:KZ4:BR	1:H:157:VAL:HG11	2.69	0.47
1:H:221:ARG:NH2	2:H:306:HOH:O	2.46	0.47
1:C:63:KZ4:BR	1:C:157:VAL:HG11	2.70	0.47
1:C:198:LYS:HG3	1:C:210:HIS:ND1	2.30	0.47
1:E:158:ASN:HB3	1:E:170:ARG:NH2	2.30	0.46
1:C:76:VAL:HB	1:C:186:PRO:HB3	1.96	0.46
1:D:63:KZ4:BR	1:D:157:VAL:HG11	2.71	0.46
1:C:137:VAL:HB	1:C:162:SER:OG	2.16	0.46
1:A:158:ASN:HB3	1:A:170:ARG:HH12	1.72	0.45
1:C:111:GLY:O	2:C:301:HOH:O	2.21	0.45
1:D:21:HIS:HA	1:D:22:PRO:HD2	1.76	0.45
1:D:158:ASN:CB	1:D:170:ARG:HH22	2.29	0.45
1:F:53:ALA:O	1:F:56:ILE:HG12	2.17	0.45
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.83	0.45
1:G:34:PHE:O	2:G:301:HOH:O	2.21	0.45
1:E:158:ASN:HB3	1:E:170:ARG:HH22	1.82	0.45
1:A:225:ASP:C	1:A:227:LEU:H	2.24	0.44
1:C:158:ASN:CG	1:C:170:ARG:HH22	2.25	0.44
1:D:158:ASN:OD1	1:D:172:ASP:CG	2.60	0.44
1:D:43:LYS:HE2	2:D:380:HOH:O	2.17	0.44
1:F:21:HIS:HA	1:F:22:PRO:HD2	1.82	0.44
1:A:144:GLU:HA	1:A:157:VAL:HB	2.00	0.44
1:H:219:LEU:HD23	1:H:219:LEU:HA	1.81	0.44
1:B:138:LYS:NZ	1:B:140:GLU:HA	2.32	0.44
1:D:104:THR:HB	2:D:390:HOH:O	2.16	0.43
1:F:201:ASP:OD2	1:F:206:ASN:ND2	2.39	0.43
1:G:63:KZ4:BR	1:G:157:VAL:HG11	2.72	0.43
1:F:63:KZ4:BR	1:F:157:VAL:HG11	2.73	0.43
1:G:65:ASN:N	2:G:312:HOH:O	2.50	0.43
1:H:66:ARG:HD2	1:H:191:VAL:HG11	2.00	0.43
1:A:100:ILE:HG21	1:C:92[B]:SER:HB3	2.00	0.43
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.76	0.43
1:D:156:ASP:OD1	1:F:170:ARG:HD2	2.18	0.43
1:G:133:GLN:NE2	2:G:303:HOH:O	2.26	0.43
1:D:219:LEU:O	2:D:301:HOH:O	2.21	0.43
1:A:198:LYS:HA	1:A:198:LYS:HD2	1.89	0.43
1:E:63:KZ4:BR	1:E:157:VAL:HG11	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:ARG:NE	1:E:156:ASP:OD1	2.46	0.43
1:C:5:LYS:HG3	1:C:6:PRO:CD	2.49	0.42
1:E:219:LEU:HD23	1:E:219:LEU:HA	1.85	0.42
1:C:154:LYS:HD3	1:C:176:THR:HG23	2.01	0.42
1:G:219:LEU:HG	1:H:192:ASP:HB3	2.01	0.42
1:B:35:GLU:OE2	2:B:302:HOH:O	2.21	0.42
1:H:5:LYS:HB3	1:H:6:PRO:CD	2.49	0.42
1:D:43:LYS:HB2	1:D:43:LYS:HE3	1.83	0.42
1:A:158:ASN:CB	1:A:170:ARG:HH12	2.31	0.41
1:C:37:LYS:NZ	2:C:311:HOH:O	2.43	0.41
1:H:5:LYS:HB3	1:H:6:PRO:HD2	2.02	0.41
1:C:11:LYS:HB2	1:C:11:LYS:HE3	1.79	0.41
1:F:192:ASP:O	1:F:213:ALA:HA	2.19	0.41
1:G:7:ASP:OD1	1:G:32:LYS:NZ	2.52	0.41
1:H:26:GLU:O	1:H:43:LYS:N	2.43	0.41
1:E:66:ARG:HD2	1:E:191:VAL:HG11	2.03	0.41
1:B:43:LYS:HA	1:B:205:SER:O	2.21	0.41
1:H:158:ASN:ND2	2:H:313:HOH:O	2.53	0.41
1:G:192:ASP:O	1:G:213:ALA:HA	2.22	0.40
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.78	0.40
1:C:66:ARG:HD3	2:C:380:HOH:O	2.20	0.40
1:F:220:PRO:HG3	2:F:396:HOH:O	2.22	0.40
1:B:164:GLU:C	1:B:166:GLY:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/255 (84%)	210 (98%)	4 (2%)	0	100	100
1	B	214/255 (84%)	211 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	214/255 (84%)	210 (98%)	4 (2%)	0	100	100
1	D	216/255 (85%)	211 (98%)	5 (2%)	0	100	100
1	E	213/255 (84%)	213 (100%)	0	0	100	100
1	F	214/255 (84%)	212 (99%)	2 (1%)	0	100	100
1	G	214/255 (84%)	212 (99%)	2 (1%)	0	100	100
1	H	215/255 (84%)	214 (100%)	1 (0%)	0	100	100
All	All	1714/2040 (84%)	1693 (99%)	21 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/217 (85%)	183 (100%)	1 (0%)	81	88
1	B	184/217 (85%)	184 (100%)	0	100	100
1	C	188/217 (87%)	188 (100%)	0	100	100
1	D	185/217 (85%)	185 (100%)	0	100	100
1	E	186/217 (86%)	185 (100%)	1 (0%)	81	88
1	F	185/217 (85%)	185 (100%)	0	100	100
1	G	184/217 (85%)	183 (100%)	1 (0%)	81	88
1	H	185/217 (85%)	185 (100%)	0	100	100
All	All	1481/1736 (85%)	1478 (100%)	3 (0%)	87	93

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	ARG
1	E	3	VAL
1	G	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	21	HIS
1	C	38	GLN
1	C	206	ASN
1	C	210	HIS
1	C	212	HIS
1	D	210	HIS
1	E	21	HIS
1	F	210	HIS
1	G	38	GLN
1	H	158	ASN
1	H	210	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KZ4	G	63	1	22,23,24	2.90	6 (27%)	28,32,34	2.39	7 (25%)
1	KZ4	E	63	1	22,23,24	2.86	7 (31%)	28,32,34	2.39	8 (28%)
1	KZ4	C	63	1	22,23,24	2.95	6 (27%)	28,32,34	2.53	7 (25%)
1	KZ4	D	63	1	22,23,24	2.95	7 (31%)	28,32,34	2.43	7 (25%)
1	KZ4	H	63	1	22,23,24	2.82	7 (31%)	28,32,34	2.31	7 (25%)
1	KZ4	F	63	1	22,23,24	2.90	7 (31%)	28,32,34	2.38	7 (25%)
1	KZ4	B	63	1	22,23,24	2.84	7 (31%)	28,32,34	2.44	7 (25%)
1	KZ4	A	63	1	22,23,24	2.95	8 (36%)	28,32,34	2.64	8 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KZ4	G	63	1	-	3/10/29/30	0/2/2/2
1	KZ4	E	63	1	-	4/10/29/30	0/2/2/2
1	KZ4	C	63	1	-	4/10/29/30	0/2/2/2
1	KZ4	D	63	1	-	4/10/29/30	0/2/2/2
1	KZ4	H	63	1	-	4/10/29/30	0/2/2/2
1	KZ4	F	63	1	-	4/10/29/30	0/2/2/2
1	KZ4	B	63	1	-	3/10/29/30	0/2/2/2
1	KZ4	A	63	1	-	4/10/29/30	0/2/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	KZ4	CA2-C2	-11.15	1.36	1.48
1	C	63	KZ4	CA2-C2	-11.07	1.36	1.48
1	D	63	KZ4	CA2-C2	-11.07	1.36	1.48
1	G	63	KZ4	CA2-C2	-10.86	1.36	1.48
1	F	63	KZ4	CA2-C2	-10.83	1.36	1.48
1	E	63	KZ4	CA2-C2	-10.72	1.36	1.48
1	B	63	KZ4	CA2-C2	-10.52	1.37	1.48
1	H	63	KZ4	CA2-C2	-10.50	1.37	1.48
1	F	63	KZ4	CG2-CB2	3.89	1.54	1.46
1	B	63	KZ4	CG2-CB2	3.83	1.53	1.46
1	E	63	KZ4	CG2-CB2	3.81	1.53	1.46
1	D	63	KZ4	CG2-CB2	3.77	1.53	1.46
1	C	63	KZ4	CG2-CB2	3.76	1.53	1.46
1	H	63	KZ4	CG2-CB2	3.71	1.53	1.46
1	G	63	KZ4	CG2-CB2	3.68	1.53	1.46
1	A	63	KZ4	CG2-CB2	3.64	1.53	1.46
1	D	63	KZ4	C2-N3	-3.54	1.31	1.40
1	H	63	KZ4	C2-N3	-3.53	1.31	1.40
1	G	63	KZ4	C2-N3	-3.52	1.31	1.40
1	B	63	KZ4	C2-N3	-3.50	1.31	1.40
1	F	63	KZ4	C2-N3	-3.49	1.32	1.40
1	A	63	KZ4	C2-N3	-3.46	1.32	1.40
1	C	63	KZ4	C2-N3	-3.43	1.32	1.40
1	E	63	KZ4	C2-N3	-3.36	1.32	1.40
1	C	63	KZ4	CA2-N2	-3.32	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	KZ4	CA2-N2	-3.20	1.31	1.38
1	E	63	KZ4	CA2-N2	-3.14	1.31	1.38
1	H	63	KZ4	CA2-N2	-3.08	1.32	1.38
1	D	63	KZ4	CA2-N2	-3.07	1.32	1.38
1	G	63	KZ4	CA2-N2	-3.07	1.32	1.38
1	B	63	KZ4	CA2-N2	-3.02	1.32	1.38
1	G	63	KZ4	CB2-CA2	-3.02	1.32	1.35
1	F	63	KZ4	CA2-N2	-2.92	1.32	1.38
1	D	63	KZ4	CB2-CA2	-2.86	1.32	1.35
1	B	63	KZ4	CB2-CA2	-2.81	1.32	1.35
1	F	63	KZ4	CB2-CA2	-2.79	1.32	1.35
1	A	63	KZ4	CB2-CA2	-2.74	1.32	1.35
1	C	63	KZ4	CB2-CA2	-2.72	1.32	1.35
1	H	63	KZ4	CB2-CA2	-2.67	1.32	1.35
1	E	63	KZ4	CB2-CA2	-2.60	1.32	1.35
1	F	63	KZ4	OH-CZ	2.30	1.41	1.36
1	B	63	KZ4	BR-CE1	2.27	1.94	1.89
1	E	63	KZ4	OH-CZ	2.27	1.40	1.36
1	G	63	KZ4	BR-CE1	2.26	1.94	1.89
1	C	63	KZ4	OH-CZ	2.23	1.40	1.36
1	B	63	KZ4	OH-CZ	2.21	1.40	1.36
1	H	63	KZ4	BR-CE1	2.20	1.94	1.89
1	E	63	KZ4	BR-CE1	2.19	1.94	1.89
1	D	63	KZ4	BR-CE1	2.14	1.94	1.89
1	F	63	KZ4	BR-CE1	2.13	1.94	1.89
1	D	63	KZ4	OH-CZ	2.12	1.40	1.36
1	A	63	KZ4	O2-C2	-2.08	1.18	1.23
1	A	63	KZ4	C1-N2	2.08	1.35	1.32
1	H	63	KZ4	OH-CZ	2.04	1.40	1.36
1	A	63	KZ4	OH-CZ	2.02	1.40	1.36

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	KZ4	O2-C2-CA2	-9.83	124.75	131.02
1	C	63	KZ4	O2-C2-CA2	-9.33	125.07	131.02
1	D	63	KZ4	O2-C2-CA2	-8.63	125.51	131.02
1	B	63	KZ4	O2-C2-CA2	-8.63	125.51	131.02
1	E	63	KZ4	O2-C2-CA2	-8.50	125.60	131.02
1	G	63	KZ4	O2-C2-CA2	-8.49	125.60	131.02
1	F	63	KZ4	O2-C2-CA2	-7.93	125.96	131.02
1	H	63	KZ4	O2-C2-CA2	-7.86	126.00	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	KZ4	CA2-C2-N3	5.94	108.49	103.50
1	D	63	KZ4	CA2-C2-N3	5.58	108.19	103.50
1	G	63	KZ4	CA2-C2-N3	5.51	108.12	103.50
1	H	63	KZ4	CA2-C2-N3	5.50	108.12	103.50
1	C	63	KZ4	CA2-C2-N3	5.43	108.06	103.50
1	E	63	KZ4	CA2-C2-N3	5.34	107.98	103.50
1	F	63	KZ4	CA2-C2-N3	5.31	107.96	103.50
1	B	63	KZ4	CA2-C2-N3	5.26	107.92	103.50
1	F	63	KZ4	N3-C1-N2	-4.15	108.21	111.48
1	B	63	KZ4	N3-C1-N2	-4.02	108.31	111.48
1	D	63	KZ4	N3-C1-N2	-3.90	108.41	111.48
1	C	63	KZ4	N3-C1-N2	-3.90	108.41	111.48
1	E	63	KZ4	N3-C1-N2	-3.81	108.48	111.48
1	A	63	KZ4	N3-C1-N2	-3.61	108.64	111.48
1	G	63	KZ4	N3-C1-N2	-3.45	108.76	111.48
1	H	63	KZ4	N3-C1-N2	-3.38	108.82	111.48
1	F	63	KZ4	CG2-CB2-CA2	-3.16	126.11	129.87
1	H	63	KZ4	CG2-CB2-CA2	-3.10	126.18	129.87
1	G	63	KZ4	CA1-CB1-SG1	-3.09	107.80	114.40
1	C	63	KZ4	CA1-CB1-SG1	-3.06	107.85	114.40
1	F	63	KZ4	CA1-CB1-SG1	-3.01	107.97	114.40
1	B	63	KZ4	CA1-CB1-SG1	-2.80	108.41	114.40
1	G	63	KZ4	CE2-CZ-CE1	2.80	120.18	118.07
1	B	63	KZ4	CA2-N2-C1	2.77	107.97	105.80
1	E	63	KZ4	CA2-N2-C1	2.76	107.96	105.80
1	H	63	KZ4	CA1-CB1-SG1	-2.69	108.65	114.40
1	D	63	KZ4	CA1-CB1-SG1	-2.66	108.72	114.40
1	D	63	KZ4	CE2-CZ-CE1	2.65	120.07	118.07
1	A	63	KZ4	BR-CE1-CZ	-2.60	117.38	119.38
1	A	63	KZ4	CE2-CZ-CE1	2.60	120.03	118.07
1	D	63	KZ4	CG2-CB2-CA2	-2.57	126.82	129.87
1	F	63	KZ4	CA2-N2-C1	2.56	107.81	105.80
1	B	63	KZ4	CE2-CZ-CE1	2.50	119.95	118.07
1	C	63	KZ4	CA2-N2-C1	2.47	107.73	105.80
1	E	63	KZ4	CA1-CB1-SG1	-2.44	109.18	114.40
1	A	63	KZ4	CA1-CB1-SG1	-2.41	109.24	114.40
1	H	63	KZ4	CA2-N2-C1	2.40	107.67	105.80
1	D	63	KZ4	CA2-N2-C1	2.34	107.63	105.80
1	H	63	KZ4	CE2-CZ-CE1	2.32	119.82	118.07
1	E	63	KZ4	CG2-CB2-CA2	-2.31	127.11	129.87
1	C	63	KZ4	CG2-CB2-CA2	-2.25	127.19	129.87
1	C	63	KZ4	CE2-CZ-CE1	2.21	119.74	118.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	KZ4	CE2-CZ-CE1	2.21	119.73	118.07
1	G	63	KZ4	CA2-N2-C1	2.20	107.52	105.80
1	G	63	KZ4	CG2-CB2-CA2	-2.19	127.26	129.87
1	A	63	KZ4	CA2-N2-C1	2.17	107.50	105.80
1	E	63	KZ4	CE2-CZ-CE1	2.15	119.69	118.07
1	A	63	KZ4	CG2-CB2-CA2	-2.13	127.33	129.87
1	E	63	KZ4	CA3-N3-C2	2.02	128.10	123.67
1	B	63	KZ4	CA3-N3-C2	2.01	128.08	123.67

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63	KZ4	C3-CA3-N3-C2
1	B	63	KZ4	C3-CA3-N3-C2
1	B	63	KZ4	C2-CA2-CB2-CG2
1	C	63	KZ4	C3-CA3-N3-C2
1	D	63	KZ4	C3-CA3-N3-C2
1	E	63	KZ4	C3-CA3-N3-C2
1	F	63	KZ4	C3-CA3-N3-C2
1	F	63	KZ4	C2-CA2-CB2-CG2
1	G	63	KZ4	C3-CA3-N3-C2
1	H	63	KZ4	C3-CA3-N3-C2
1	H	63	KZ4	C2-CA2-CB2-CG2
1	B	63	KZ4	N2-CA2-CB2-CG2
1	E	63	KZ4	N2-CA2-CB2-CG2
1	F	63	KZ4	N2-CA2-CB2-CG2
1	H	63	KZ4	N2-CA2-CB2-CG2
1	D	63	KZ4	N2-CA2-CB2-CG2
1	G	63	KZ4	N2-CA2-CB2-CG2
1	D	63	KZ4	C2-CA2-CB2-CG2
1	E	63	KZ4	C2-CA2-CB2-CG2
1	C	63	KZ4	N2-CA2-CB2-CG2
1	G	63	KZ4	C2-CA2-CB2-CG2
1	A	63	KZ4	N2-CA2-CB2-CG2
1	C	63	KZ4	C2-CA2-CB2-CG2
1	C	63	KZ4	C3-CA3-N3-C1
1	F	63	KZ4	C3-CA3-N3-C1
1	H	63	KZ4	C3-CA3-N3-C1
1	A	63	KZ4	C2-CA2-CB2-CG2
1	A	63	KZ4	C3-CA3-N3-C1
1	D	63	KZ4	C3-CA3-N3-C1

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Mol	Chain	Res	Type	Atoms
1	E	63	KZ4	C3-CA3-N3-C1

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	63	KZ4	1	0
1	E	63	KZ4	1	0
1	C	63	KZ4	1	0
1	D	63	KZ4	1	0
1	H	63	KZ4	1	0
1	F	63	KZ4	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	218/255 (85%)	-0.05	11 (5%) 34 36	11, 34, 57, 87	2 (0%)
1	B	216/255 (84%)	-0.12	7 (3%) 50 53	13, 33, 54, 75	2 (0%)
1	C	218/255 (85%)	-0.10	6 (2%) 55 57	13, 34, 55, 91	2 (0%)
1	D	220/255 (86%)	-0.04	8 (3%) 46 48	14, 34, 58, 92	2 (0%)
1	E	215/255 (84%)	-0.21	6 (2%) 55 57	12, 33, 56, 73	2 (0%)
1	F	216/255 (84%)	-0.12	5 (2%) 61 64	13, 34, 54, 89	2 (0%)
1	G	218/255 (85%)	0.03	9 (4%) 41 43	14, 37, 63, 86	2 (0%)
1	H	216/255 (84%)	0.01	6 (2%) 55 57	14, 38, 61, 83	3 (1%)
All	All	1737/2040 (85%)	-0.08	58 (3%) 49 51	11, 35, 58, 92	17 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	227	LEU	7.4
1	C	227	LEU	6.2
1	A	4	ILE	5.8
1	D	220	PRO	5.4
1	H	158	ASN	5.3
1	D	227	LEU	5.3
1	G	224	MET	5.0
1	A	220	PRO	4.8
1	A	227	LEU	4.7
1	D	228	TYR	4.5
1	C	220	PRO	4.5
1	H	3	VAL	4.4
1	A	150[A]	ASP	4.3
1	A	228	TYR	3.9
1	B	158	ASN	3.9
1	B	4	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	4	ILE	3.8
1	G	4	ILE	3.7
1	A	170	ARG	3.5
1	E	3	VAL	3.5
1	D	3	VAL	3.4
1	D	224	MET	3.3
1	A	225	ASP	3.3
1	G	220	PRO	3.2
1	F	3	VAL	3.2
1	C	225	ASP	3.2
1	C	224	MET	3.2
1	B	165	GLY	3.2
1	C	184	GLN	3.2
1	C	4	ILE	3.1
1	B	44	VAL	3.0
1	F	21	HIS	3.0
1	G	184	GLN	2.7
1	F	100	ILE	2.7
1	B	220	PRO	2.7
1	F	4	ILE	2.7
1	D	170	ARG	2.6
1	D	225	ASP	2.5
1	D	4	ILE	2.5
1	G	226	GLU	2.5
1	G	225	ASP	2.4
1	E	158	ASN	2.3
1	A	20	GLY	2.3
1	A	226	GLU	2.2
1	B	3	VAL	2.2
1	F	221	ARG	2.2
1	G	158	ASN	2.2
1	H	165	GLY	2.2
1	E	30	LEU	2.2
1	A	21	HIS	2.2
1	E	21	HIS	2.2
1	E	172	ASP	2.1
1	B	221	ARG	2.1
1	G	21	HIS	2.1
1	A	11	LYS	2.1
1	H	220	PRO	2.0
1	E	4	ILE	2.0
1	H	206	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KZ4	A	63	22/23	0.97	0.06	22,28,34,50	0
1	KZ4	C	63	22/23	0.97	0.06	21,27,33,48	0
1	KZ4	D	63	22/23	0.97	0.07	24,27,31,53	0
1	KZ4	G	63	22/23	0.97	0.06	24,32,36,54	0
1	KZ4	H	63	22/23	0.97	0.07	27,34,39,55	0
1	KZ4	F	63	22/23	0.98	0.06	22,30,35,54	0
1	KZ4	B	63	22/23	0.98	0.07	23,29,35,50	0
1	KZ4	E	63	22/23	0.98	0.07	22,30,35,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.